Quantum Discord of an Arbitrary State of Two Qubits

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Calculation of the quantum discord requires to find the minimum of the quantum conditional entropy $S(\rho^{AB}|\{\Pi_k^B\})$ over all measurements on the subsystem B. In this paper, we provide a simple relation for the conditional entropy as the difference of two Shannon entropies. The relation is suitable for calculation of the quantum discord in the sense that it can by used to obtain the quantum discord for some classes of two-qubit states, without the need for minimization. We also present an analytical procedure of optimization and obtain conditions under which the quantum conditional entropy of a general two-qubit state is stationary. The presented relation is also used to find a tight upper bound on the quantum discord.

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I. INTRODUCTION

Entanglement is the specific feature of quantum systems which reveals that complete information about parts of a composite system does not include complete information of the whole system [1, 2]. However, this is not the only weird character of a quantum system. For instance, the collapse of one part of a non-entangled bipartite quantum system after a measurement on the other part is another feature unique to quantum systems. The quantity that captures this feature is the quantum discord [3, 4]. The key idea of the concept of quantum discord is the superposition principle and the vanishing of discord shown to be a criterion for quantum to classical transition [3]. Furthermore, quantum discord has a simple interpretation in thermodynamics and has been used in analyzing the power of a quantum Maxwell's demon [5]. It has also been employed in the study of pure quantum states as a resource and performance of deterministic quantum computation with one pure qubit [6]. The authors of Refs. [7, 8] showed that non-classical correlations other than entanglement can be responsible for the quantum computational efficiency of deterministic quantum computation with one pure qubit [6] and brought this obscured correlation measure to the spot light zone. After this discovery, quantum discord becomes one of the most frequent topics of researches in the field of quantum information theory. Indeed, quantum discord is the difference between two classically equivalent definitions of mutual information in the quantum mechanics language. In mathematical sense, discord could be obtained by eliminating the whole of classical correlation from the total correlation measured by mutual information, by means of the most destructive measurement on the one party of the system. Mutual information of a bipartite system can be written as

$$I(\rho^{AB}) = S(\rho^A) + S(\rho^B) - S(\rho^{AB}), \tag{1}$$

where ρ^A and ρ^B refer to the reduced density matrices of the subsystems A and B, respectively, ρ^{AB} is the density matrix of the system as the whole, and $S(\rho) = -\mathrm{Tr}(\rho \log_2 \rho)$ is the Von Neumann entropy. The classical correlation between the parts of a bipartite system can be obtained by use of the measurement-base conditional density operator and can be written as [3]

$$C_B(\rho^{AB}) = \sup_{\{\Pi_k^B\}} \{S(\rho^A) - S(\rho^A|\{\Pi_k^B\})\}. \tag{2}$$

Here the maximum is taken over all projective measurement $\{\Pi_k^B\}$ on the subsystem B [3], and $S(\rho^A|\{\Pi_k^B\}) = \sum_k p_k S(\rho_k^A)$ is the conditional entropy of the subsystem A, with $\rho_k^A = \mathrm{Tr}_B((\mathbb{I}^A \otimes \Pi_k^B)\ \rho^{AB}\ (\mathbb{I}^A \otimes \Pi_k^B))/p_k$ as the post-measurement state of the subsystem A and $p_k = \mathrm{Tr}(\rho^{AB}(\mathbb{I}^A \otimes \Pi_k^B))$ being the probability of the k-th outcome. The maximum performed in Eq. (2) can be taken also over all the positive operator valued measures (POVM) [4] and these two definitions give in general inequivalent results. Accordingly, discord can be calculated as follows

$$D_B(\rho^{AB}) = I(\rho^{AB}) - C_B(\rho^{AB}). \tag{3}$$

However, one can swap the role of the subsystems A and B to obtain $D_A(\rho^{AB})$, which is not equal to $D_B(\rho^{AB})$ in general. In this paper we only consider $D_B(\rho^{AB})$ and hence ignore the subscript B in the following.

The optimization procedure involved in the calculation of quantum discord prevents one to write an analytical expression for quantum discord even for simple two-qubit systems. Quantum discord is analytically computed only for a few families of states including the Bell-diagonal states [9, 10], two-qubit X states [11, 12], two-qubit rank-2 states [13], a class of rank-2 states of $4 \otimes 2$ systems [14], and Gaussian states of the continuous variable systems [15]. Moreover, based on the optimization of the conditional entropy, an algorithm to calculate the quantum discord of the two-qubit states is presented in [16]. It is also important to have some computable bounds on the quantum discord and some authors have obtained such bounds [17, 18].

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In this paper, we consider two-qubit states and obtain a simple relation for the quantum conditional entropy $S(\rho^{AB}|\{\Pi_k^B\})$ as the difference of two Shannon entropies. This form of the conditional entropy enables one to calculate its minimum for some classes of two-qubit states, without any minimization procedure. An analytical progress in the minimization of the conditional entropy of a general two-qubit state is also presented. Moreover, we obtain a tight upper bound on the quantum discord of an arbitrary two-qubit state and show that such obtained upper bound satisfy the stationary conditions of the conditional entropy, when we restrict the measurement direction to a special subspace of $\mathbb{R}^3$.

The paper is organized as follows. In section II, we consider a general two-qubit system and present a simple relation for the quantum conditional entropy. In this section, we also evaluate the quantum discord for some classes of states, and present a tight upper bound on the discord of a general two-qubit state. Section III is devoted to the optimization procedure. An analytical conditions under which the conditional entropy is stationary is presented in this section. The paper is concluded in section IV with a brief discussion.

II. CONDITIONAL ENTROPY AND QUANTUM DISCORD OF TWO-QUBIT STATES

A general two-qubit state can be written in the Hilbert-Schmidt representation as

$$\rho^{AB}=\frac{1}{4}\left(\mathbb{I}\otimes\mathbb{I}+\vec{x}\cdot\sigma\otimes\mathbb{I}+\mathbb{I}\otimes\vec{y}\cdot\sigma+\sum_{i,j=1}^{3}t_{ij}\sigma_i\otimes\sigma_j\right). \tag{4}$$

Here $\mathbb{I}$ stands for the identity operator, $\{\sigma_i\}_{i=1}^3$ are the standard Pauli matrices, $\vec{x}$ and $\vec{y}$ are coherence vectors of the subsystems A and B, respectively, and $T=(t_{ij})$ is the correlation matrix. Therefore, to each state ρ^{AB} we associate the triple $\{\vec{x},\vec{y},T\}$. Since quantum correlations are invariant under local unitary transformation, i.e. under transformations of the form $(U_1\otimes U_2)\rho^{AB}(U_1^\dagger\otimes U_2^\dagger)$ with $U_1,U_2\in SU(2)$, we can, without loss of generality, restrict our considerations to some representative class of the states described by less number of parameters [19]. Under such transformations, the triple $\{\vec{x},\vec{y},T\}$ transforms as

$$\vec{x}\to O_1\vec{x},\qquad \vec{y}\to O_2\vec{y},\qquad T\to O_1TO_2^t, \tag{5}$$

where O_i's corresponds to U_i's via $U_i(\vec{a}\cdot\vec{\sigma})U_i^\dagger=(O_i\vec{a})\cdot\vec{\sigma}$ [19]. In view of this, any state of the two-qubit system can be written as $(U_1\otimes U_2)\rho^{AB}(U_1^\dagger\otimes U_2^\dagger)$, where ρ^{AB} belongs to the representative class. In the following we will consider a representative class such that T is diagonal, namely $T=\mathrm{diag}\{t_1,t_2,t_3\}$. Concerning this representative class, a general state of two-qubit system can be parameterized by nine real parameters $\vec{x}=(x_1,x_2,x_3)^t$, $\vec{y}=(y_1,y_2,y_3)^t$, and $T=\mathrm{diag}\{t_1,t_2,t_3\}$, where t denotes transposition. Accordingly, in the computational basis $\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$, a general state ρ^{AB} of this representative class takes the following form

$$\rho^{AB}=\frac{1}{4}\begin{pmatrix}\rho_{11} & y_1-iy_2 & x_1-ix_2 & t_1-t_2\\ y_1+iy_2 & \rho_{22} & t_1+t_2 & x_1-ix_2\\ x_1+ix_2 & t_1+t_2 & \rho_{33} & y_1-iy_2\\ t_1-t_2 & x_1+ix_2 & y_1+iy_2 & \rho_{44}\end{pmatrix}, \tag{6}$$

where

$$\rho_{11}=1+x_3+y_3+t_3,\quad \rho_{22}=1+x_3-y_3-t_3,$$
$$\rho_{33}=1-x_3+y_3-t_3,\quad \rho_{44}=1-x_3-y_3+t_3.$$

Now let us turn our attention on the von Neumann measurement on the subsystem B. A general such measurement can be written as

$$\Pi_k^B=U|k\rangle\langle k|U^\dagger, \tag{7}$$

where $\{|k\rangle\langle k|\}_{k=0}^1$ is the von Neumann projection operators in the standard basis of the subsystem B, and $U\in SU(2)$. An arbitrary element of $SU(2)$ can be factorized as [20]

$$U=\Omega_2\Omega_1, \tag{8}$$

with Ω_2 and Ω_1 defined by

$$\Omega_2=\begin{pmatrix}\cos\frac{\theta}{2} & -\mathrm{e}^{-i\phi}\sin\frac{\theta}{2}\\ \mathrm{e}^{i\phi}\sin\frac{\theta}{2} & \cos\frac{\theta}{2}\end{pmatrix},\quad \Omega_1=\begin{pmatrix}\mathrm{e}^{i\eta/2} & 0\\ 0 & \mathrm{e}^{-i\eta/2}\end{pmatrix}, \tag{9}$$

for $0\le\theta\le\pi$, $0\le\phi\le2\pi$, and $0\le\eta\le\pi$. Therefor, we get $\Pi_k^B=\Omega_2|k\rangle\langle k|\Omega_2^\dagger=|\sigma\cdot\hat{n}_k\rangle\langle\sigma\cdot\hat{n}_k|$ where $\hat{n}_0=-\hat{n}_1=\hat{n}$, with $\hat{n}=(\sin\theta\cos\phi,\sin\theta\sin\phi,\cos\theta)^t$. This, explicitly, shows that only two independent parameters θ and ϕ are needed to characterize a general von Neumann measurement on the two-qubit systems. We can also write these orthogonal projections in the Bloch representation as

$$\Pi_k^B=\frac{1}{2}\left(\mathbb{I}+\hat{n}_k\cdot\sigma\right),\qquad k=0,1. \tag{10}$$

Therefore $\hat{n}_0$ and $\hat{n}_1$ are coherence vectors of Π_0^B and Π_1^B, respectively. For further use, we calculate the expression $\Pi_k^B\sigma_j\Pi_k^B$ for $k=0,1$ and $j=1,2,3$, i.e.

$$\begin{aligned}\Pi_k^B\sigma_j\Pi_k^B&=|\sigma\cdot\hat{n}_k\rangle\langle\sigma\cdot\hat{n}_k|\sigma_j|\sigma\cdot\hat{n}_k\rangle\langle\sigma\cdot\hat{n}_k|\\&=\mathrm{Tr}\big(\Pi_k^B\sigma_j\big)\Pi_k^B=(\hat{n}_k)_j\Pi_k^B.\end{aligned} \tag{11}$$

Now we are in the position to perform the von Neumann measurement $\{\Pi_k^B\}_{k=0}^1$ on the qubit B. This transforms the total state ρ^{AB} to the ensemble $\{p_k,\rho_k^{AB}\}_{k=0}^1$ such that

$$\rho_k^{AB}=\frac{1}{p_k}(\mathbb{I}\otimes\Pi_k^B)\rho^{AB}(\mathbb{I}\otimes\Pi_k^B), \tag{12}$$

with $p_k=\mathrm{Tr}[(\mathbb{I}\otimes\Pi_k^B)\rho^{AB}(\mathbb{I}\otimes\Pi_k^B)]$. By using Eqs. (4) and (10) in (12) and invoking relation (11) we get

$$\rho_k^{AB}=\rho_k^A\otimes\Pi_k^B, \tag{13}$$

where

$$\rho_k^A = \frac{1}{2}\left(\mathbb{I} + \vec{\tilde{x}}_k \cdot \sigma\right), \tag{14}$$

is the post-measurement state of the qubit A, associated to the measurement result k with the corresponding probability

$$p_k = \frac{1}{2}\left(1 + \vec{y}^t \hat{n}_k\right). \tag{15}$$

In Eq. (14), the post-measurement coherence vector $\vec{\tilde{x}}_k$ is defined by

$$\vec{\tilde{x}}_k = \frac{\vec{x} + T\hat{n}_k}{1 + \vec{y}^t \hat{n}_k}. \tag{16}$$

The quantum conditional entropy with respect to the above measurement is defined by

$$S(\rho^A|\{\Pi_k^B\}) = p_0 S(\rho_0^A|\{\Pi_k^B\}) + p_1 S(\rho_1^A|\{\Pi_k^B\}). \tag{17}$$

Using

$$\frac{1}{2}\left(1 \pm |\vec{\tilde{x}}_k|\right) = \frac{1}{4p_k}\left(2p_k \pm |\vec{x} + T\hat{n}_k|\right), \tag{18}$$

as the eigenvalues of ρ_k^A, for $k = 1, 2$, and after some calculations we obtain the following relation for the conditional entropy

$$S(\rho^A|\{\Pi_k^B\}) = h_4(\vec{w}) - h_2(p_0). \tag{19}$$

Above, and throughout this paper, $h_2(x)$ denotes the binary Shannon entropy [21] defined by

$$h_2(x) = -x\log_2 x - (1-x)\log_2(1-x), \tag{20}$$

and $h_m(q_1, \cdots, q_m) = -\sum_{i=1}^m q_i \log_2 q_i$ is the Shannon entropy of the probabilities $\{q_1, \cdots, q_m\}$. In particular, $h_4(\vec{w}) = -\sum_{i=1}^4 w_i \log_2 w_i$ is the Shannon entropy of the probabilities

$$w_{1,2} = \frac{2p_0 \pm |\vec{x} + T\hat{n}|}{4}, \quad w_{3,4} = \frac{2p_1 \pm |\vec{x} - T\hat{n}|}{4}. \tag{21}$$

Note that under the transformation $\hat{n} \to -\hat{n}$, corresponding to $\theta \to \pi - \theta$ and $\phi \to \phi \pm \pi$, the probabilities (15) and (21) transform as $p_0 \leftrightarrow p_1$, $w_1 \leftrightarrow w_3$ and $w_2 \leftrightarrow w_4$, leaving therefore the conditional entropy invariant. On the other hand, if we perform local unitary transformation (5) on the density matrix, the probabilities (15) and (21), and hence the conditional entropy do not change provided we perform the transformation $\hat{n} \to O_2\hat{n}$. This implies that if we find $\hat{n}^*$ as the optimal measurement for a given state ρ^{AB} of the representative class, one can obtain the optimal one for any state $\tilde{\rho}^{AB} = (U_1 \otimes U_2)\rho^{AB}(U_1^\dagger \otimes U_2^\dagger)$, just by the transformation $\hat{n}^* \to O_2\hat{n}^*$.

Now the aim is to minimize the above conditional entropy. Before we give a general procedure for optimization, we give below some special classes of states for which the quantum discord can be evaluated without the need for any optimization.

Bell-diagonal states.— As the first example, let us consider the Bell-diagonal states, i.e. states with the maximal marginal entropies. For this three-parameters class of states we have $\vec{x} = 0$, $\vec{y} = 0$ and $T = \mathrm{diag}\{t_1, t_2, t_3\}$. In this particular case we have

$$p_0 = p_1 = \frac{1}{2}, \quad w_{1,2} = w_{3,4} = \frac{1}{4}\left(1 \pm |T\hat{n}|\right), \tag{22}$$

which leads to the following simple form for the conditional entropy (19)

$$S(\rho^A|\{\hat{n}\}) = h_2\left(\frac{1 + |T\hat{n}|}{2}\right), \tag{23}$$

Clearly, the minimum of the above equation occurs for $\max|T\hat{n}| = \max\sqrt{\hat{n}^t T^t T\hat{n}}$, which is achieved when $\hat{n}$ is an eigenvector of $T^t T$ corresponding to the largest eigenvalue $t_{\max}^2$

$$\min S(\rho^A|\{\hat{n}\}) = h_2\left(\frac{1 + t_{\max}}{2}\right), \tag{24}$$

where we have defined

$$t_{\max} = \max\{|t_1|, |t_2|, |t_3|\}. \tag{25}$$

Therefore, the discord is obtained as follows

$$S(\rho^{AB}) = 1 - h_4(\mu_1, \mu_2, \mu_3, \mu_4) + h_2\left(\frac{1 + t_{\max}}{2}\right),$$

where $\{\mu_i\}_{i=1}^4$ are eigenvalues of ρ^{AB} given by

$$\mu_{1,2} = \frac{1}{4}\left(1 \pm t_1 \pm t_2 - t_3\right), \quad \mu_{3,4} = \frac{1}{4}\left(1 \pm t_1 \mp t_2 + t_3\right).$$

This is in agreement with the result obtained by Luo in [9].

States with $T^t\vec{x} = 0$ and $\vec{y} = 0$.— For the second class we consider states such that $\vec{y} = 0$ and $\vec{x}$ belongs to the kernel of T^t, i.e. $T^t\vec{x} = 0$. For this class of states we get

$$|x + T\hat{n}| = |x - T\hat{n}| = \sqrt{x^2 + \hat{n}^t T T\hat{n}}, \tag{26}$$

and therefore

$$p_0 = p_1 = \frac{1}{2}, \qquad w_{1,2} = w_{3,4} = \frac{1}{4}\left(1 \pm |\vec{x} + T\hat{n}|\right). \tag{27}$$

This leads to

$$S(\rho^A|\{\hat{n}\}) = h_2\left(\frac{1 + |x + T\hat{n}|}{2}\right). \tag{28}$$

The minimum of the above equation occurs whenever $|x + T\hat{n}| = \sqrt{x^2 + \hat{n}^t T^t T\hat{n}}$ takes its maximum value. This happens when $\hat{n}$ is an eigenvector of $T^t T$ corresponding to the largest eigenvalue $t_{\max}^2$, therefore

$$\min S(\rho^A|\{\hat{n}\}) = h_2\left(\frac{1 + \sqrt{x^2 + t_{\max}^2}}{2}\right), \tag{29}$$

where $t_{\max}$ is defined by Eq. (25). Note that the condition $T^t\vec{x}=0$ requires that $t_i x_i = 0$ for $i=1,2,3$. Hence if we take, without loss of generality, $|t_1|\geq|t_2|\geq|t_3|\geq 0$ and set $\vec{y}=0$, then the states corresponding to this class can be obtained from the general form of Eq. (6) as:
(i) States with $x_1=x_2=x_3=0$. This corresponds to the Bell-diagonal states where we have studied them, separately.
(ii) States with $x_1=x_2=t_3=0$. This corresponds to a three-parameter subclass of the so-called X states. In this case, the discord is obtained as

$$S(\rho^{AB}) = 1 - h_4(\mu_1,\mu_2,\mu_3,\mu_4) + h_2\left(\frac{1+\sqrt{t_1^2+x_3^2}}{2}\right),$$

where $\{\mu_i\}_{i=1}^4$ are eigenvalues of ρ^{AB} given by

$$\mu_{1,2} = \frac{1}{4}\left(1\pm\sqrt{(t_1+t_2)^2+x_3^2}\right),$$
$$\mu_{3,4} = \frac{1}{4}\left(1\pm\sqrt{(t_1-t_2)^2+x_3^2}\right).$$

(iii) States with $x_1=t_2=t_3=0$. This corresponds to a three-parameter subclass of the zero-discord states.
(iv) States with $t_1=t_2=t_3=0$. This also corresponds to a three-parameter subclass of the zero-discord states.

Interestingly, the above two examples motivate us to introduce an upper bound for the quantum discord. Let $\mathcal{R}$ be the subspace of $\mathbb{R}^3$ spanned by $T^t\vec{x}$ and $\vec{y}$, i.e. $\mathcal{R}=\mathrm{span}\{T^t\vec{x},\vec{y}\}$, and let $\mathcal{R}^\perp$ denotes the orthogonal complement of $\mathcal{R}$, i.e. the set of all vectors in $\mathbb{R}^3$ that are orthogonal to every element of $\mathcal{R}$. Hence we have $\mathcal{R}+\mathcal{R}^\perp=\mathbb{R}^3$.

Theorem 1 *The conditional entropy (19) is bounded from above as*

$$\min_{\{\Pi_k^B\}} S(\rho^A|\{\Pi_k^B\}) \leq h_2\left(\frac{1+\sqrt{x^2+t_0^2}}{2}\right), \quad (30)$$

where $x=|\vec{x}|$, and

$$t_0^2 = \max_{\hat{e}_0\in\mathcal{R}^\perp} \hat{e}_0^t T^t T \hat{e}_0. \quad (31)$$

Accordingly, the classical correlation and the quantum discord have the following lower and upper bounds, respectively

$$C(\rho^{AB}) \geq S(\rho^A) - h_2\left(\frac{1+\sqrt{x^2+t_0^2}}{2}\right), \quad (32)$$

$$Q(\rho^{AB}) \leq S(\rho^B) - S(\rho^{AB}) + h_2\left(\frac{1+\sqrt{x^2+t_0^2}}{2}\right) \quad (33)$$

Proof Let us concern about all measurement directions $\hat{e}_0$ living in $\mathcal{R}^\perp$, i.e. $\vec{y}^t\hat{e}_0=0$, $(T^t\vec{x})^t\hat{e}_0=0$; then

$$|x+T\hat{e}_0| = |x-T\hat{e}_0| = \sqrt{x^2+\hat{e}_0^t TT\hat{e}_0}, \quad (34)$$

and

$$p_0=p_1=\frac{1}{2}, \quad w_{1,2}=w_{3,4}=\frac{1}{4}\left(1\pm|\vec{x}+T\hat{e}_0|\right). \quad (35)$$

Therefore

$$\begin{aligned}\min_{\hat{n}\in\mathbb{R}^3} S(\rho^A|\{\hat{n}\}) &\leq \min_{\hat{e}_0\in\mathcal{R}^\perp} S(\rho^A|\{\hat{e}_0\}) \\ &= \min_{\hat{e}_0\in\mathcal{R}^\perp} h_2\left(\frac{1+\sqrt{x^2+\hat{e}_0^t TT^t\hat{e}_0}}{2}\right) \\ &= h_2\left(\frac{1+\sqrt{x^2+t_0^2}}{2}\right),\end{aligned} \quad (36)$$

where $t_0^2=\max \hat{e}_0^t T^t T\hat{e}_0$ with the maximum taken over all unit vectors $\hat{e}_0\in\mathcal{R}^\perp$. Evidently, if two vectors $T^t\vec{x}$ and $\vec{y}$ be nonzero and linearly independent then $\dim\mathcal{R}^\perp=1$, so that the unit vector $\hat{e}_0\in\mathcal{R}^\perp$ is unique. Otherwise $\dim\mathcal{R}^\perp>1$, so we can choose $\hat{e}_0\in\mathcal{R}^\perp$ such that $t_0^2=\max_{\hat{e}_0\in\mathcal{R}^\perp}\hat{e}_0^t T^t T\hat{e}_0$, giving a tighter bound. This completes the proof of (30). Using Eq. (30) in Eqs. (2) and (3), we obtain the desired bounds (32) and (33), respectively.

Remarkably, the above bound is tight in the sense that for all states that $\mathcal{R}^\perp=\mathbb{R}^3$, the bound is achieved. This happens, for example, when $\vec{x}=\vec{y}=0$ or $T^t\vec{x}=\vec{y}=0$. In these cases t_0^2 becomes the largest eigenvalue of T^tT and $\hat{e}_0$ is the corresponding eigenvector. As we will show in the example below, it may happens $\mathcal{R}^\perp\neq\mathbb{R}^3$ but the upper bound (30) is achieved. In these cases the absolute minimum of the conditional entropy happens for directions in $\mathcal{R}^\perp\subseteq\mathbb{R}^3$. Latter, we show that the above upper bound corresponds to the stationary point of the conditional entropy when we restrict ourselves to the solutions in $\mathcal{R}^\perp$.

Recently an upper bound for the quantum discord is obtained in [17] as $Q(\rho^{AB})\leq S(\rho^B)$. A comparison of this with the upper bound presented in (33) shows that for all states for which $S(\rho^{AB})-h_2\left(\frac{1+\sqrt{x^2+t_0^2}}{2}\right)>0$, our bound is stronger.

As an illustrative example let us consider a two-parameter class of states discussed in [22]

$$\rho^{AB}(a,b)=\frac{1}{2}\begin{pmatrix} a & 0 & 0 & a \\ 0 & 1-a-b & 0 & 0 \\ 0 & 0 & 1-a+b & 0 \\ a & 0 & 0 & a\end{pmatrix}, \quad (37)$$

where $0\leq a\leq 1$ and $a-1\leq b\leq 1-a$. The discord of this state is [22]

$$Q(\rho^{AB}(a,b)) = \min\{a,q\}, \quad (38)$$

where

$$q = \frac{a}{2}\log_2\left[\frac{4a^2}{(1-a)^2-b^2}\right] - \frac{b}{2}\log_2\left[\frac{(1+b)(1-a-b)}{(1-b)(1-a+b)}\right]$$
$$- \frac{\sqrt{a^2+b^2}}{2}\log_2\left[\frac{1+\sqrt{a^2+b^2}}{1-\sqrt{a^2+b^2}}\right]$$
$$+ \frac{1}{2}\log_2\left[\frac{4((1-a)^2-b^2)}{(1-b^2)(1-a^2-b^2)}\right]. \quad (39)$$

For this state we get

$$\vec{x} = -\vec{y} = \begin{pmatrix} 0 \\ 0 \\ -b \end{pmatrix}, \quad T = \begin{pmatrix} a & 0 & 0 \\ 0 & -a & 0 \\ 0 & 0 & 2a-1 \end{pmatrix}. \quad (40)$$

Clearly, $T^t\vec{x} = -(2a-1)\vec{y}$, so that for all values of a and $b \neq 0$ we have $\mathcal{R} = \mathrm{span}\{\vec{y}\}$. Therefore an arbitrary element of $\mathcal{R}^\perp$ can be written as $\hat{e}_0 = (\cos\phi, \sin\phi, 0)^t$. In this case we get $\hat{e}_0^t T^t T \hat{e}_0 = a^2$, which is independent of ϕ, so that $t_0 = a^2$. This means that every vector in the two-dimensional subspace $\mathcal{R}^\perp$, corresponding to the xy-plane, gives the desired upper bound. Therefore, we obtain

$$\min_{\hat{e}_0\in\mathcal{R}^\perp} S(\rho^A|\{\hat{e}_0\}) = h_2\left(\frac{1+\sqrt{a^2+b^2}}{2}\right), \quad (41)$$

and

$$S(\rho^A) = S(\rho^B) = h_2\left(\frac{1+b}{2}\right), \quad (42)$$
$$S(\rho^{AB}) = h_3\left(a, \frac{1-a-b}{2}, \frac{1-a+b}{2}\right), \quad (43)$$

where $h_3(\mu_1,\mu_2,\mu_3) = -\sum_{i=1}^3 \mu_i \log_2 \mu_i$. After some calculations we find that the inequality (33) leads to

$$Q(\rho^{AB}(a,b)) \leq q, \quad (44)$$

where q is defined in Eq. (39). A comparison of this with Eq. (38) shows that for some region of parameters, namely when $q \leq a$, our upper bound is tight. Figs. 1 and 2 illustrate this fact. These figures also reveal that for this class of states our bound is stronger than the upper bound of Ref. [17].

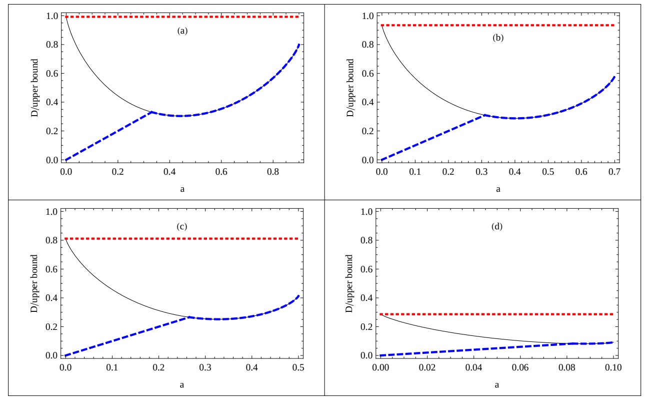

FIG. 1. (Color online) Quantum discord [dashed-blue lines], our upper bound [solid-black lines], and the upper bound of Ref. [17] [dotted-red lines] are plotted versus a for the state $\rho^{AB}(a,b)$ with: (a) $b = 0.1$, (b) $b = 0.3$, (c) $b = 0.5$, and (d) $b = 0.9$.

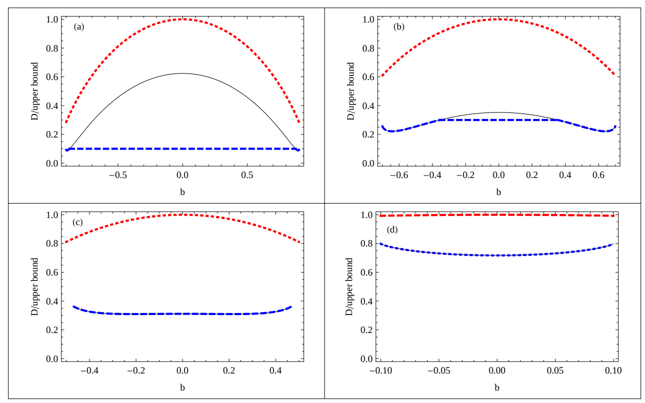

FIG. 2. (Color online) Quantum discord [dashed-blue lines], our upper bound [solid-black lines], and the upper bound of Ref. [17] [dotted-red lines] are plotted versus b for the state $\rho^{AB}(a,b)$ with: (a) $a = 0.1$, (b) $a = 0.3$, (c) $a = 0.5$ (d) $a = 0.9$. In the cases (c) and (d), our upper bound completely coincide with the quantum discord.

III. OPTIMIZATION

In this section we present an analytical procedure for optimization of the conditional entropy for a general two-qubit state. We also provide examples for which one can obtain the the minimum, analytically. In order to determine the minimum of the conditional entropy (19), we have to calculate its derivatives with respect to θ and ϕ. To do this we need to calculate derivatives of the probabilities given by Eqs. (15) and (21) with respect to θ and ϕ. For instance, their derivative with respect to θ are as follows

$$\frac{\partial p_{0,1}}{\partial\theta} = \pm\frac{1}{2}\hat{n}^t_{,\theta}\,\vec{y}, \quad (45)$$
$$\frac{\partial w_{1,2}}{\partial\theta} = \frac{1}{4}\hat{n}^t_{,\theta}\,\left[\vec{y} \pm T^t\hat{Z}^+\right], \quad (46)$$
$$\frac{\partial w_{3,4}}{\partial\theta} = \frac{1}{4}\hat{n}^t_{,\theta}\,\left[-\vec{y} \pm T^t\hat{Z}^-\right], \quad (47)$$

with

$$\hat{Z}^+ = \frac{T\hat{n}+\vec{x}}{|T\hat{n}+\vec{x}|}, \qquad \hat{Z}^- = \frac{T\hat{n}-\vec{x}}{|T\hat{n}-\vec{x}|}, \quad (48)$$

and the unit vector $\hat{n}_{,\theta}$ is defined by

$$\hat{n}_{,\theta} = \frac{\partial \hat{n}}{\partial \theta} = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta)^t. \qquad (49)$$

Evidently $\hat{n}\cdot\hat{n}_{,\theta} = 0$. By defining the nonunit vector $\tilde{n}_{,\phi}$ by

$$\tilde{n}_{,\phi} = \frac{\partial \hat{n}}{\partial \phi} = (-\sin\theta\sin\phi, \sin\theta\cos\phi, 0)^t, \qquad (50)$$

orthogonal to both $\hat{n}$ and $\hat{n}_{,\theta}$, we get a similar equations for the derivatives of the probabilities with respect to ϕ, but now $\hat{n}_{,\theta}$ is replaced by $\tilde{n}_{,\phi}$. Using the above equations, we arrive at the following conditions for the stationary conditions $\partial S(\rho^A|\{\Pi_k^B\})/\partial\theta = \partial S(\rho^A|\{\Pi_k^B\})/\partial\phi = 0$

$$\hat{n}_{,\theta}^t\, \vec{A} = 0, \qquad \tilde{n}_{,\phi}^t\, \vec{A} = 0, \qquad (51)$$

where $\vec{A}$ is a vector defined by

$$\vec{A} = \left[\log_2 \frac{w_1 w_2 p_1^2}{w_3 w_4 p_0^2}\right]\vec{y} + \left[\log_2 \frac{w_1}{w_2}\right] T^t \hat{Z}^+ + \left[\log_2 \frac{w_3}{w_4}\right] T^t \hat{Z}^-. \qquad (52)$$

Conditions (51) can be written also as

$$\hat{n}_{\perp}^t\, \vec{A} = 0, \qquad (53)$$

where $\hat{n}_\perp$ is any vector perpendicular to $\hat{n}$, i.e. $\hat{n}_\perp^t \hat{n} = 0$. Equation (53) shows that the stationary points of $S(\rho^A|\{\Pi_k^B\})$ happens whenever the vector $\vec{A}$ is in the direction of $\hat{n}$. If we proceed the optimization process by using the Lagrange multiplier λ, having $\hat{n}^t\hat{n} = 1$ as a constraint, we find for the stationary condition $\mathrm{d}\left[S(\rho^A|\{\Pi_k^B\}) - \lambda(\hat{n}^t\hat{n} - 1)\right] = 0$ the following relation

$$\vec{A} = A\hat{n}, \qquad (54)$$

where $\vec{A}$ is defined in Eq. (52), and A is given by

$$A = -\left[\log_2 \frac{w_1}{w_2}\right] \vec{x}^t \hat{Z}^+ + \left[\log_2 \frac{w_3}{w_4}\right] \vec{x}^t \hat{Z}^- - 4S(\rho^A|\{\Pi_k^B\}) - \left[\log_2 \frac{w_1 w_2 w_3 w_4}{p_0^2 p_1^2}\right], \qquad (55)$$

The stationary condition (54) is equivalent to that given by Eq. (53) in the sense that both conditions require that in the extremum points, the vector $\vec{A}$ should be directed to $\hat{n}$. Unfortunately, these conditions do not have simple solutions, for $\vec{A}$ as well as A depends also on $\hat{n}$. Moreover, knowing the extremum points of the conditional entropy is not enough to establish its minimum, and we need, in addition, to evaluate the conditional entropy in the extremum points. Below we exemplify these conditions for some particular cases where we have already obtained the minimum of the conditional entropy without optimization.

Bell-diagonal states.— For this class of states we already showed that the optimal measurement lies in the direction of the eigenvector of T^tT, corresponding to the largest eigenvalue. In this case the vector $\vec{A}$ takes the following form

$$\vec{A} = \frac{2}{|T\hat{n}|}\left[\log_2 \frac{1+|T\hat{n}|}{1-|T\hat{n}|}\right] T^tT\hat{n}. \qquad (56)$$

It is clear that the condition (53) leads to $\hat{n}_\perp^t T^tT\hat{n} = 0$, which has solutions when $\hat{n}$ is an eigenvector of T^tT. But the 3×3 matrix T^tT has three nonnegative eigenvalues $\{t_1^2, t_2^2, t_3^2\}$ corresponding to the eigenvectors $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$. Therefore, the conditional entropy in the stationary points is obtained as

$$S(\rho^A|\{\hat{e}_k\}) = h_2\left(\frac{1+|t_k|}{2}\right), \quad \text{for} \quad k = 1,2,3. \qquad (57)$$

Simple evaluation shows that the minimum of the above equation happens when $|t_k|$ corresponds to the largest eigenvalue of $\sqrt{T^tT}$.

States with $T\vec{x} = 0$ and $\vec{y} = 0$.— In this case the vector $\vec{A}$ takes the following form

$$\vec{A} = \frac{2}{|T\hat{n}+\vec{x}|}\left[\log_2 \frac{1+|T\hat{n}+\vec{x}|}{1-|T\hat{n}+\vec{x}|}\right] T^tT\hat{n}. \qquad (58)$$

Again the condition (53) leads to $\hat{n}_\perp^t T^tT\hat{n} = 0$, which has solutions when $\hat{n}$ is an eigenvector of T^tT. Therefore, in the stationary directions $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$ we get

$$S(\rho^A|\{\hat{e}_k\}) = h_2\left(\frac{1+\sqrt{x^2+t_k^2}}{2}\right), \quad \text{for} \quad k = 1,2,3. \qquad (59)$$

Again, evaluation shows that the minimum of the above entropy happens when t_k^2 corresponds to the largest eigenvalue of T^tT.

Examples above show that the stationary condition given in Eq. (53) gives us, in general, more than one solution for the measurement direction $\hat{n}$, and we have to find the optimal one by further evaluations.

Let us mention here that the upper bound expressed in the theorem 1 can be actually obtained from a special class of solutions of the stationary condition (53), namely the one restricted to the subspace $\mathcal{R}^\perp$ of $\mathbb{R}^3$. To show this, we have to show that if the measurement direction $\hat{e}_0$, living in the subspace $\mathcal{R}^\perp$ of $\mathbb{R}^3$, satisfy the stationary condition (53) then the upper bound (30) is obtained as the minimum of the conditional entropy. Concerning about all measurement directions $\hat{e}_0$ living in $\mathcal{R}^\perp$; then

$$S(\rho^A|\{\hat{e}_0\}) = h_2\left(\frac{1+|x+T\hat{e}_0|}{2}\right). \qquad (60)$$

and

$$\vec{A} = \frac{2}{|T\hat{e}_0+\vec{x}|}\left[\log_2 \frac{1+|T\hat{e}_0+\vec{x}|}{1-|T\hat{e}_0+\vec{x}|}\right] T^tT\hat{e}_0, \qquad (61)$$

where by assumption, $\hat{e}_0$ should satisfy the stationary condition (53). Now if $\dim\mathcal{R} = 2$, i.e. when two vectors $T^t\vec{x}$ and $\vec{y}$ are nonzero and independent, then the

stationary condition (53) can be expressed as

$$\vec{y}^t \vec{A} = 0, \qquad (T^t \vec{x})^t \vec{A} = 0. \tag{62}$$

Using (61) in the above conditions, we get

$$\vec{y}^t T^t T \hat{e}_0 = 0, \qquad (T^t \vec{x})^t T^t T \hat{e}_0 = 0, \tag{63}$$

where implies that $T^t T \hat{e}_0 \in \mathcal{R}^\perp$. But since $\dim \mathcal{R}^\perp = 1$, therefore $T^t T \hat{e}_0$ should be in the direction of $\hat{e}_0$, or equivalently $\hat{e}_0$ should be an eigenvector of $T^t T$ corresponding to the eigenvalue t_0^2. On the other hand, if one or both of vectors $T^t \vec{x}$ and $\vec{y}$ be zero or they are nonzero but linearly dependent, then $1 < \dim \mathcal{R}^\perp \leq 3$. In this case the two conditions given by Eq. (63) are no longer independent and $\hat{e}_0$ is not unique. In any case we get

$$\min_{\hat{e}_0 \in \mathcal{R}^\perp} S(\rho^A | \{\hat{e}_0\}) = h_2 \left(\frac{1 + \sqrt{x^2 + t_0^2}}{2} \right), \tag{64}$$

where t_0^2 is defined by Eq. (31). Equation (64) gives the conditional entropy in the stationary point $\hat{e}_0$, restricted to the subspace $\mathcal{R}^\perp \in \mathbb{R}^3$, and is equal to the upper bound for the conditional entropy given by Eq. (30). Evidently, if $\dim \mathcal{R} = 0$, or if the conditional entropy evaluated in $\mathcal{R} \in \mathbb{R}^3$ does not be smaller than Eq. (64), then the minimum given by Eq. (64) gives the absolute minimum of the conditional entropy and the upper bound (30) is achieved.

IV. CONCLUSION

All difficulties in calculating the quantum discord arise from the difficulty in finding the minimum of the quantum conditional entropy $S(\rho^{AB} | \{\Pi_k^B\})$ over all measurements on the subsystem B. In this work, we have presented a simple relation for the quantum conditional entropy of a two-qubit system, as the difference of two Shannon entropies. Using it, we have obtained the quantum discord for a class of states for which the conditions $T^t \vec{x} = 0$ and $\vec{y} = 0$ are satisfied. This class of states includes the Bell-diagonal states, a three-parameter subclass of X states, and some zero-discord states. For these states, it is shown that the quantum conditional entropy reduces to the binary Shannon entropy, so that in minimizing the conditional entropy we encountered with the simple problem of minimizing binary Shannon entropy. We have shown that such obtained relation for the conditional entropy can be used to present a tight upper bound on the quantum discord. We have exemplified this bound for a two-parameter class of states and show that in some regions of the parameters our bound is saturated. A general procedure of optimization of the conditional entropy is also given, and by some examples it is shown that it can be used to calculate the quantum discord for some classes of states, analytically. It is also shown that such obtained upper bound on the conditional entropy is actually a solution of the stationary conditions of the conditional entropy, when we restrict the measurement direction to a subspace of $\mathbb{R}^3$. We hope that our results provide further insight into the problem of quantum discord. The method presented in this paper can be generalized to higher dimensional systems.

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[1] A. Einstein, B. Podolsky and N. Rosen, Phys. Rev. **47**, 777 (1935)

[2] E. Schrödinger, Naturwiss. **23**, 807 (1935).

[3] H. Ollivier and W. H. Zurek, Phys. Rev. Lett. **88**, 017901 (2001).

[4] L. Henderson, and V. Vedral, J. Phys. A **34**, 6899 (2001).

[5] W. H. Zurek, Phys. Rev. A **67**, 012320 (2003).

[6] Knill E. and Laflamme R., Phys. Rev. Lett. **81**, 5672(1998).

[7] A. Datta, A. Shaji and C.M. Caves, Phys. Rev. Lett. **100** 050502 (2008); and A. Datta and S. Gharibian, Phys. Rev. A **79**, 042325(2009).

[8] B. P. Lanyon, M. Barbieri, M. P. Almeida, and A. G. White, Phys. Rev. Lett. **101** 200501 (2008).

[9] S. Luo, Phys. Rev. A **77**, 042303 (2008).

[10] M. D. Lang, and C. M. Caves, Phys. Rev. Lett. **105**, 150501 (2010).

[11] M. Ali, A. R. P. Rau, and G. Alber, Phys. Rev. A **81**, 042105 (2010).

[12] Q. Chen, C. Zhang, S. Yu, X. X. Yi, and C. H. Oh, Phys. Rev. A **84**, 042313 (2011).

[13] M. Shi, W. Yang, F. Jiang, and J. Du, J. Phys. A: Math. Theor. **44**, 415304 (2011).

[14] L. X. Cen, X. Q. Li, J. Shao, and Y. J. Yan, Phys. Rev. A **83**, 054101 (2011).

[15] G. Adesso and A. Datta, Phys. Rev. Lett. **105**, 030501 (2010).

[16] D. Girolami, and G. Adesso, Phys. Rev. A **83**, 052108 (2011).

[17] Z. Xi, X-M Lu, X. Wang, and Y. Li, J. Phys. A: Math. Theor. **44**, 375301 (2011).

[18] S. Yu, C. Zhang, Q. Chen, C. H. Oh, arXiv:1102.1301 (2011).

[19] R. Horodecki, and M. Horodecki, Phys. Rev. A **54**, 1838 (1996).

[20] R. Gilmore, *Lie Groups, Lie Algebras, and Some of Their Applications* (John Wiley & Sons, New York, USA, 1974).

[21] M. A. Nielsen, and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, UK, 2000).

[22] A. Al-Qasimi, and D. F. V. James, Phys. Rev. A **83**, 032101 (2011).